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AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE A	ND DATES COVERED
4. TITLE AND SUBTITLE	November 30, 2000	Final Ol	5. FUNDING NUMBERS
Using flux information at improve a groundwater flo		ries to	DAAH04-96-1-0046
6. AUTHOR(S) David Genereux, James S	Saiers, Carl Bolster		
7. PERFORMING ORGANIZATION NAME	ES(S) AND ADDRESS(ES)		8. PERFORMING ORGANIZATION
Department of Geology Florida International Uni Miami, FL 33199	Note: PI now Marine, Eart	h, & Atmos. State Univ.,	REPORT NUMBER
9. SPONSORING / MONITORING AGEN	NCY NAME(S) AND ADDRESS(ES)		10. SPONSORING / MONITORING
U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27	7709_2211		ARO 35552.12-EV
Research Thangle Lark, IVE 27	707-2211		DAH
11. SUPPLEMENTARY NOTES The views, opinions and/or find an official Department of the A	lings contained in this report a army position, policy or decision.	are those of the authon, unless so design	nor(s) and should not be construed as nated by other documentation.
12a. DISTRIBUTION / AVAILABILITY STA	ATEMENT		12 b. DISTRIBUTION CODE
Approved for public release; di	stribution unlimited.		
13. ABSTRACT (Maximum 200 words)			
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1. Appendices

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2. Research Problem

2.1. Overview

During the past three decades, groundwater flow models have been applied with increasing frequency to address environmental issues related to water quality and water supply [Bredehoeft et al., 1982; Anderson and Woessner, 1992]. Numerical models for groundwater flow solve a partial differential equation, together with the associated initial and boundary conditions, for the temporal and spatial distribution in hydraulic head. The location and magnitude of groundwater sources and sinks and parameter values for aquifer storage, hydraulic conductivity, and thickness govern the calculated hydraulic head distribution. In many instances, field-based estimates of aquifer parameters are unavailable, and, as a result, parameters are determined from model calibration. Model calibration traditionally has involved identifying the values of the model parameters that minimize the differences between model-computed and field-measured hydraulic heads. Results of studies that employ nonlinear regression techniques have demonstrated that inverse solutions derived solely from observations on hydraulic head are often ill posed [Anderman et al., 1996; Keating and Bahr, 1998]. That is, the calibration process fails to accurately quantify aquifer properties because the model parameters are insensitive to the hydraulic head measurements or because high correlation between fitted parameters prevents identification of a unique optimal parameter set [Yeh, 1986; Hill et al., 1998].

Several researchers have proposed that groundwater inverse problems can be constrained better if other types of hydrologic data, in addition to data on hydraulic heads, are utilized as the calibration targets. For synthetic aquifers characterized by idealized transmissivity fields, Poeter and Hill [1997] showed that observations on groundwater flow to surface-water bodies could be used with head measurements to obtain unique parameter estimates in cases when head data alone were insufficient to constrain the inverse problem. D'agnese et al. [1996] calibrated a steady-state flow model of the Death Valley aquifer system with a combination of head measurements and flow observations from groundwater-fed springs; however, the authors did not address whether or not the supplemental information on spring discharges changed parameter estimates relative to an inverse solution based only on head data. Like flow measurements, data on the subsurface migration of dissolved tracers have been used to strengthen model calibration [Gorelick et al., 1983; Krabbenhoft, 1990; Keidser and Rosbjerg, 1991; Barlebo et al., 1996; Anderman and Hill, 1999]. Keating and Bahr [1998] reported problems with solution nonuniqueness when using head data to calibrate a groundwater model for a small watershed, but were able to eliminate a number of plausible flow configurations by coupling data on dissolved calcium concentrations with head data in the calibration of a flow and solute transport model. In a similar fashion, Anderman et al. [1996] observed that inclusion of data on boron transport through a sand-and-gravel aquifer decreased the correlation between parameters of a particletracking model and thus increased the uniqueness of the inverse solutions.

Although a few published reports suggest that information on groundwater fluxes and solute

concentrations serves to improve model calibration, the number of studies is inadequate to thoroughly evaluate this conclusion, especially as it applies to complex geologic systems. Consequently, the response of optimal parameter estimates, parameter correlation, and parameter uncertainty to attempts to constrain the inverse problem by supplementing head observations with other data types is not well established for field problems. Furthermore, studies that center only on flow-model calibration far outnumber those that report calibration results in combination with groundwater-flow predictions. Owing to this lack of evaluations of calibrated models, there is no clear evidence that flow predictions based on parameter estimated from inversions with multiple calibration targets (e.g., heads and water fluxes or heads and solute concentrations) are more accurate than flow predictions based on parameters estimated from inversions with heads as the sole calibration target.

In this work, we systematically examine the value of using groundwater flux and solute concentration measurements in coordination within nonlinear regression techniques to estimate parameters that describe transient groundwater flow through a limestone aquifer. We construct a three-dimensional groundwater flow and solute transport model for a portion of Florida's Biscayne Aquifer, and, in a sequence of inverse simulations, we calibrate this model with data on (1) hydraulic heads, (2) hydraulic heads and groundwater fluxes to canals, and (3) hydraulic heads, groundwater fluxes, and pore-water concentrations of chloride, a naturally occurring conservative tracer. We then use the parameterizations obtained from the three calibrations to predict groundwater-flow dynamics measured during a time interval outside the calibration period. Our results demonstrate that best-fit values of the parameters for storage, hydraulic conductivity, and canal-bed conductance are sensitive to the types of data used in the calibration process and that the accuracy of the groundwater flux predictions, and, to a lesser extent, the accuracy of the head predictions, depend on the combination of data types used in the calibration process.

2.2. Methods

2.2.1. Study Site

The study site is located about 50 km southwest of Miami, along the eastern boundary of Everglades National Park (ENP; Figure 1). Climate is subtropical, with a hot, humid wet season (May through October) and a mild dry season (November through April). Average annual temperature in Homestead is 23° C and average annual precipitation over ENP was 141 cm from 1951 to 1985.

The field site was chosen in part because of it is of major local and national environmental interest. The Frog Pond area and nearby lands (Figure 1) are among the most controversial sites for water management in the U.S., largely because of the often competing demands of ecosystem preservation and restoration within ENP and flood protection in residential and agricultural lands immediately to the east of the ENP. Our work is related to these water management issues insofar as it quantifies the value of various data types in model calibration, and hydrologic models used by government agencies are important water management tools at the study site.

Ground surface elevations in the area vary from approximately 3 m near Homestead to zero at the coastline (elevations referenced to U.S. National Geodetic Vertical Datum, or NGVD). ENP lands within the model domain are very low relief marl prairies dominated by sawgrass (*Cladium*

jamaicense) and muhly grass (Muhlenbergia filipes), with a few isolated tree islands or hammocks. Taylor Slough (Figure 1) is an elongate, low-lying zone that served as the natural drainage way for the area; such sloughs contain abundant macrophytes, including water lily (Numphaea odorata), submerged aquatics, and periphyton mats. Farm lands to the east of ENP produce mainly beans, tomatoes, and squash, along with a wide variety of minor ornamental and orchard crops.

The area is underlain by the Biscayne Aquifer, an extremely conductive unconfined aquifer with a hydraulic conductivity of 7,600 m/d [Genereux and Guardiario, 1998]. The hydraulic conductivity value is a large-scale average, based on a canal drawdown test in which the response of the aquifer was monitored while water management structures were manipulated to rapidly lower the water level in the L-31W canal about 30 cm [Genereux and Guardiario, 1998]. This sort of large-scale K value is well suited to our assumption of lateral homogeneity in hydraulic conductivity; the area responding to the drawdown test was actually a significant fraction of the model domain in the present study. Using a similar approach at a site about 30 km north, Chin [1991] obtained a large-scale estimate of K only 3% lower than that of Genereux and Guardiaro [1998], indicating the Biscayne Aquifer is homogeneous across fairly large distances when the measurement area or volume is large. There is of course abundant small-scale (cm to m) heterogeneity in the aquifer that is averaged over such large-scale K values.

The wedge-shaped Biscayne Aquifer covers most of Dade and Broward counties in southeast Florida and thickens toward the coast. Thickness varies from about 12 m in the northwest corner of Figure 1 to 24 m in the southeast. Within our model domain the Biscayne consists of two formations: the Miami Limestone Formation and the underlying Fort Thompson Formation [Fish and Stewart, 1991]. Small zones of a third formation (the coralline Key Largo Formation) interfinger with the other two formations in the southeast portion of Figure 1 [Fish and Stewart, 1991]. The Miami Limestone consists mainly of bryozoan, pelletal, and solitic limiestone, while the Fort Thompson has abundant coquina and other shell-rich limestone interbedded with denser, fine-grained freshwater limestones. There is extensive secondary solution in both formations (more so in the marine than freshwater limestones in the Fort Thompson). Formation thicknesses were estimated by kriging available borehole data. The Miami Limestone ranges in thickness from 4 m to 6 m in the model area, and the Fort Thompson from 7 to 13 m (thicker toward the southeast).

The C-111 and L-31W canals were completed in 1967 and 1971, respectively. Both canals penetrate the Biscayne Aquifer through the Miami Limestone. Flow in the canals is to the south, toward Florida Bay at the southern tip of the peninsula. C-111 is the larger of the two canals, having been designed as the principal flood control canal for a large portion of south-central Dade County. Design discharges at the structures on C-111 (all gated spillways; Fig 2) increase southward from 17.8 m³/s at S-176 to 68 m³/s at S-197. Canal width increases significantly toward the south, from about 23 m near S-176 to 48.5 m near the overpass for U.S. Highway 1 at typical water level elevations. Maximum depth increases from about –4.2 m NGVD to –5.2 m NGVD between the two sites.

The L-31W borrow canal is significantly smaller, being about 17 m wide at typical water level elevations; maximum depth is about -4.1 m NGVD. Structures S-174 (a gated spillway) and S-

175 (a gated three-barrel culvert) were both designed for 14.2 m³/s. A levee built of canal dredge material runs along the eastern side of L-31W. The canal itself carries water to Taylor Slough, a low-lying natural drainage feature which meanders south-southwest through the sawgrass marsh. Pump station S-332 (which has a capacity of 13.2 m³/s) sits almost in the center of Taylor Slough, and pumps water westward from the L-31W canal into the slough. Ideally, this arrangement should allow water levels in the canal to be kept low for flood protection (required mainly for agricultural lands east of L-31 W) while water deliveries needed for ecological reasons are made to ENP through Taylor slough, using S-332.

2.2.2. Field Measurements of Heads, Groundwater Fluxes, and Chloride Concentrations Observations on porewater chloride concentrations, hydraulic head, and groundwater exchange with the L-31 W canal were recorded over a 2-year period beginning in January 1997 and were used separately or in combination to calibrate and test the flow and transport model. We collected groundwater from 7 wells screened with the Miami Limestone and canal water at each of the water-control structures on a bi-weekly basis (Figure 1). These samples were analyzed by ion chromatography for concentrations of chloride and other major anions. We obtained data on hydraulic head at 14 groundwater wells (Figure 1) and data on canal stage at the water control structures from public-domain databases maintained by the South Florida Water Management District, the United States Geological Survey, and Everglades National Park. We converted the stage measurements at S-174 and S-175 structures to discharge estimates with pre-established rating curves, and we used these discharge estimates in coordination with discharge measurements from the S-332 pump station to calculate total daily water fluxes between the aquifer and L-31W by

$$Q_g = -(\Delta s - Q_{S174} + Q_{S175} + Q_{S332} + (E - P) * A)$$

where Q_g is the groundwater discharge into the L-31 canal, Q_{S174} and Q_{S175} are canal discharges at the S-174 spillway and S-175 culvert, respectively, Q_{S332} is the water discharged from the S-332 pump station, E is the daily evaporation rate, P is the daily precipitation rate, A is the canal area, and Δs is the change in storage in the canal. Evaporation from the canal was assumed equal to evaporation from a Class A evaporation pan located at Tamiami Ranger Station. P represents a weighted average determined from rain gages located at five stations in the study area. (Details on zonation of rainfall are provided in section 2.2.3.)

2.2.3. Model Description

We calculated the distribution in hydraulic heads and groundwater discharges to canals with MODFLOW, a three-dimensional finite-difference model for nonsteady groundwater flow, and we simulated coupled groundwater flow and chloride transport by linking MODFLOW with MT3D, a three-dimensional model for advective-dispersive transport. The finite-difference grid for the flow and transport calculations consisted one layer to represent the Miami Limestone formation and a second layer to represent the underlying Fort Thompson Formation. We estimated the spatial variability in layer thicknesses by kriging field data from borehole measurements. Each model layer was discretized into 48 rows and 59 columns and was designed to accommodate closer nodal spacing near the canals, where we anticipated model-computed gradients in hydraulic heads and solute concentrations to be the highest. The time-step size and stress period were set to equal 0.25 days and 1 day, respectively. Result of preliminary

simulations demonstrated that further decreases in time-step size or nodal spacing did not significantly change calculations of hydraulic head or chloride concentrations.

We oriented the finite-difference grid such that each corner of the grid corresponded with the location of a hydraulic-head observation well (Figure 1), and we specified the hydraulic heads along the straight-line boundary segments between each grid corner by linear interpolation. Our measurements reveal that vertical head gradients are negligible in the Frog Pond [Genereux and Guardiario, 1998]; therefore, we assigned equal boundary-head values to both model layers. We assumed that porewater concentrations of chloride along the boundaries of the model domain were constant and equal to 20 mg/L. This assumption is consistent with our observations that variability in porewater chloride concentrations are confined to regions near the canals, while groundwater collected in wells far from the canals exhibit little spatial or temporal variability in chloride levels.

We used MODFLOW's River Package to simulate the exchange of water between the Biscayne Aquifer and the L-31W and C-111 canals. Both the canal-bed conductance and the canal stage govern this head-dependent formulation. We assumed that each canal was characterized by a uniform conductance, but that the magnitude of conductance varied between canals. We calculated the downstream decline in canal stage by linearly interpolating between stages measured at adjacent water-control structures. We represented Taylor Slough with a single line of specified-head nodes that stretched in a southwest direction from the west side of the S-332 Pump Station to the Taylor Slough Bridge. For a given stress period, these heads were set to decrease in a linear fashion between the head value measured at the pump station to the head value measured that the bridge.

Fluxes of chloride between the canal and the surrounding aquifer were simulated with MT3D by specifying the concentration of chloride within the canal reach. Canal-water chloride concentrations were considered uniform between adjacent water-control structures and were estimated by averaging measurements of chloride concentrations recorded at adjacent upstream and downstream structures.

We accounted for the spatial variability in groundwater recharge by dividing the model domain into five recharge zones. We employed the Thiessen method to define five polygonal areas in which the perpendicular bisectors of lines joining adjacent rain gages form the boundaries of the polygons (Figure 1). Daily values of recharge for each zone were determined as the difference between the recorded rainfall for that zone and evapotranspiration. Estimates of evapotranspiration were assumed to be uniform over the Frog Pond. Evapotranspiration was determined on a daily basis by application of the Bowen ratio method to a site located along Old Ingram Highway, 2 km west of the Frog Pond. We assume that evaporation from the water table was negligible, so recharge was set to zero on days in which no rainfall was recorded.

2.2.4. Parameter Estimation

We report the results of inverse simulations in which data on heads, groundwater fluxes, and chloride concentrations were used separately or in combination to calibrate a coupled flow and transport model. Several computer programs, including UCODE [Poeter and Hill, 1999], MODFLOWP [Hill, 1992], and PEST, have been developed to solve groundwater inverse

problems. We chose PEST for this work because it is distributed with GMS, a computer program capable of processing input and output files for MODFLOW and MT3D. PEST implements a variant of the Gauss-Marquadt-Levenberg method to estimate values of parameters that minimize a weighted sum of squares objective function, calculated as

$$S(b) = \sum_{i=1}^{Nh} u_i \left(h_i - \hat{h}_i \right)^2 + \sum_{i=1}^{Nq} v_j \left(q_j - \hat{q}_j \right)^2 + \sum_{k=1}^{Nc} w_k \left(c_k - \hat{c}_k \right)^2$$
 (2)

where Nh, Nq, and Nc are the numbers of head observations, groundwater flux observations, and porewater chloride observations, \hat{h}_i , \hat{q}_j , and \hat{c}_k refer to model-simulated values of head, flux, and chloride concentration, h_i , q_j , and c_k refer to the observed values of head, flux, and chloride concentration, and u_i , v_j , and w_k , are the weights associated with the respective observation types.

The weights can be approximated as the inverse of the variances of the observation measurement errors. Components of the measurement error often are difficult to quantify, however. Consequently, variances of the observation errors are assigned subjectively and are sometimes updated based on regression results [Poeter and Hill, 1997; Hill, 1998; Hill et al., 1998]. In the work reported here, we assigned variances of 1 X 10⁻⁴ m² and 1 mg²/l² to the head measurements and chloride measurements, respectively. We used the error propagation formula outlined by Taylor [1997] to estimate the variance in the groundwater flux errors from the uncertainties in canal discharges measured at S-174, S-175, and S-332. Canal discharges at the structures are determined from rating curves established by the South Florida Water Management District; thus, the error in the discharge observation reflects the uncertainty in the stage measurement at the structure. By specifying a stage-measurement error of 1 X 10⁻⁴ m² in the error propagation formula, we estimated a value of 2.5 X 10⁷ (m³/d)² for the variance in the groundwater flux errors.

The model was calibrated with hydrologic data measured over a 195-day period that began on 2 January 1998 and ended on 9 September 1998 and included parts of the dry and wet seasons. The hydraulic conductivity and specific yield of the Miami Limestone and the canal bed conductances of L-31W and C-111 were estimated in inversions in which head alone or heads and fluxes served as the calibration targets. These four parameters were estimated together with the longitudinal dispersivity in inverse simulations in which heads, fluxes, and chloride concentrations were used simultaneously as the calibration targets.

Estimates of the remaining model parameters – the storage coefficient and hydraulic conductivity of the Fort Thompson Formation and the lateral dispersivity – were determined from field measurements or from the literature. Analysis of preliminary simulations revealed that model-calculated solutions were insensitive to changes in the storage coefficient of the Fort Thompson, so we set this parameter equal to 0.0005, which is a typical value for limestone aquifers [Freeze and Cherry, 1979]. Results of borehole flow meter tests conducted at our site demonstrate that the ratio of the hydraulic conductivity of the Miami Limestone Formation to the hydraulic conductivity of the Fort Thompson Formation equals 4.2 [Genereux and Guardiario, 1998]. We used this ratio in the calibration process to specify the Fort Thompson hydraulic conductivity as a function of the Miami Limestone hydraulic conductivity. In accordance with the work of Segol and Pinder [1976], we assume that a single value of longitudinal dispersivity is appropriate for describing dispersion in the Miami Limestone and Fort Thompson Formations, and we set the

value of the lateral dispersivity at 1/10 the value of the longitudinal dispersivity.

We assess the agreement between observed and model-calculated results with a statistical index, referred to as the model efficiency. We report model efficiencies that quantify the goodness of model fits to the head measurements (E_h) and, when appropriate, model efficiencies that quantify the goodness of model fits to the groundwater flux measurements (E_q) and to the chloride concentrations measurements (E_c) . As the equations that define each of the model efficiencies are identical in form, we present the equation for E_h only:

$$E_{h} = \frac{\sum_{i=1}^{Nh} (u_{i}h_{i} - h_{av})(u_{i}\hat{h}_{i} - \hat{h}_{av})}{\left[\sum_{i=1}^{Nh} (u_{i}h_{i} - h_{av})(u_{i}h_{i} - h_{av})\sum_{i=1}^{Nh} (u_{i}\hat{h}_{i} - \hat{h}_{av})(u_{i}\hat{h}_{i} - \hat{h}_{av})\right]^{1/2}}$$
(3)

where h_{av} and \hat{h}_{av} equal the mean value of the weighted observed heads and the mean value of the weighted model-calculated heads, respectively. A model efficiency of 1 indicates a perfect fit of the model to the data, while a model efficiency of zero indicates that the model fits the data no better than a straight line through the mean of the observations.

2.3. Results

Model calculations closely match measured heads in the inverse simulations with hydraulic heads as the sole calibrations target (Figure 2); the model efficiency for the overall fit to the head data equals 0.98. Each of the measured well hydrographs exhibits substantial fluctuation in heads, which is captured well by the model. The greatest deviation between computed and observed heads occurs at the Roblee well site, but even here, the residuals between simulated and measured values does not exceed 0.1 m and averages less than 0.05 m. We conducted the inverse simulations five times with different starting values for the four adjustable parameters. In each case, the model converged to the same optimal parameter values. Calculated parameter correlations are less than or equal to 0.32, which provides some evidence that head data alone may be sufficient to estimate unique parameter values (Table 1). All four adjustable parameters were estimated precisely from the head data. Calculations of the coefficient of variation, defined as standard error of the parameter estimate divided by the estimated parameters value, are less than 0.2 and are as low as 0.05 (Table 1). The best-fit estimates of each of the aquifer parameters appear reasonable (Table 1); however, the estimate of the Miami Limestone hydraulic conductivity is nearly a factor of two greater than value reported by Genereux and Guardiaro [1998].

Modeled results closely mimic field measurements in inverse simulations in which groundwater fluxes are used together with hydraulic heads as the calibration targets (Figure 3 and Figure 4). The model efficiencies associated with the fits to the head and flux data are 0.98 and 0.93, respectively. Despite some small discrepancies between computed and measured fluxes, the overall model-data agreement is remarkable given the large temporal variations in measured groundwater fluxes (Figure 4). In a fashion similar to the head-only calibration the coefficients of variation are uniformly small in magnitude (Table 1), indicating that the uncertainty in the parameter estimates is low. The absolute values of the parameter correlations range from 0.01 to 0.72, with the highest correlation being between the Miami Limestone hydraulic conductivity and

the L31W canal-bed conductance (Table 1). Although greater than that observed for the heads-only calibration, the maximum correlation calculated for the head-and-flux calibration is relatively low as Poeter and Hill suggest that aquifer parameters can be estimated with parameter correlations as high as 0.98.

The groundwater flux data could not be mimicked with values of the aquifer parameters obtained from the heads-only calibration; hence the addition of the flux data to the calibration drove substantial changes in the optimal values of the aquifer parameters. Changes in the values of C_{L31W} and S_y are significant, but the largest changes are associated with K_{ML} , which varies by a factor of two between the heads-only and the head-and-and flux calibrations, and C_{C111} , which varies by over an order of magnitude between the two calibrations (Table 1). These results suggest that more than one parameter set is capable of quantifying the spatial and temporal variations in hydraulic head with good success, but that a good match to the head data does not necessarily translate to accurate simulation of groundwater fluxes.

The mathematical model for coupled flow and transport accounts for much of the variation in the field measurements when heads, fluxes, and chloride concentrations are used simultaneously as the calibration targets (Figures 5, 6, and 7). The model efficiencies for the fits to the head, groundwater flux, and chloride data are 0.98, 0.91, 0.90, respectively. Comparison of these efficiency calculations to those obtained from the head-and-flux calibration reveals that the addition of the chloride data did not significantly degrade the accuracy of the simulations of head and groundwater flux. Chloride concentrations exhibit the greatest temporal variability in wells P3 and P23S, which are located east of the ENP boundary and very close to L31W. The model reproduces the overall features of the chloride breakthrough curves measured at these two wells, although it slightly underestimates the magnitude of the chloride concentrations observed in P3S.

The model also simulates the flat chloride responses measured at the four remaining monitoring wells, installed either to the west of the ENP boundary or far from L31W canal (Figure 7). The best-fit values of the flow parameter are nearly the same as those estimated from the head-and-flux calibration, and the optimal value of the longitudinal dispersivity equals 6.6 m, which closely matches the value determined for a portion of the Biscayne aquifer located east of our study site (Table 1).

- 3. Publications supported in part or in whole through this project, in reverse chronological order (boldface indicates ARO author listed in section 4) 30. Saiers, J.E., D.P. Genereux, C. Bolster, and E. Zechner. The benefit of using multiple data types in estimation of hydrogeological parameters in the Biscayne Aquifer. In preparation for submission to *Ground Water*.
- 29. **Bolster, C., D.P. Genereux, and J.E. Saiers**. Estimation of specific yield in the Biscayne Aquifer through a controlled canal drawdown test. In preparation for submission to *Ground Water*.
- 28. **Saiers, J.E**. Laboratory observations and mathematical modeling of colloid-facilitated contaminant transport in chemically heterogeneous systems. Submitted to *Water Resources Research*.

- 27. **Bolster, C. H.** and **J.E. Saiers.** Development and evaluation of a mathematical model for surface-water flow within the Shark River Slough of the Florida Everglades. Submitted to *Water Resources Research*.
- 26. **Genereux, D.P.**, and J.D.A. Guardiario. A borehole flowmeter investigation of small-scale hydraulic conductivity variation in the Biscayne Aquifer, Florida. Revised version submitted to *Water Resources Research*.
- 25. Guha, H., **J.E. Saiers**, S.C. Brooks, P. M. Jardine, and K. Jayachandran. Chromium transport, oxidation, and adsorption within β -MnO2-coated sand. *Journal of Contaminant Hydrology*, in press.
- 24. **Genereux**, **D.P.**, and I. Bandopadhyay. Numerical investigation of lake bed seepage patterns: Effects of porous medium and lake properties. *Journal of Hydrology*, in press.
- 23. Saiers, J.E., H. Guha, P.M Jardine, and S.C. Brooks. 2000. Development and evaluation of a mathematical model for the coupled transport and oxidation-reduction of chelated metals in water-saturated porous media. *Water Resources Research*, 36: 3151-3165.
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Massachusetts, May-June 1999.

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5. Inventions

None to report.

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Appendix 1: Technical interaction/exchange with US Army researchers and contractors Our participation in formal meetings organized by ARO, including presentation of research talks, included (1) the joint ARO/AFOSR meeting in Panama City, Florida, in January 1997 and (2) the ARO Terrestrial Sciences meeting at the Waterways Experiment Station (WES), Vicksburg, Mississippi, in July 1997.

The majority of technology transfer was in the form of e-mail and phone calls over the life of the project to WES and one of their contractors (the Environmental Modeling Research Lab at Brigham Young University, BYU) concerning the Groundwater Modeling System (GMS), software for modeling groundwater flow and solute transport. GMS was developed by BYU in conjunction with WES, and was used heavily in our research. Our use of the GMS resulted in identification and eventual correction of numerous software bugs, probably in part because our application was fairly demanding (it involved setting up and running inverse simulations for groundwater flow and solute transport, calibrating on different combinations of head, groundwater seepage, and chemical concentration data). Finding and resolving these problems slowed progress on our project but pointed out critical areas for improvement of the GMS. For example, a brief summary of the major problems encountered most recently (in 2000) includes:

- the specific head package within the GMS was not working properly (the GMS was not writing the MODFLOW files correctly); correction of this bug took over two weeks
- it was not possible to fit the specific yield of the aquifer in inverse simulations; this involved problems with both the GMS and PEST (separate inverse simulation software)
- there were problems with the GMS in calculating transient fluxes from the river package (a module for handling groundwater exchange with rivers)
- there were problems with the way GMS was writing the input files for MT3D (a solute transport model used in our work).

Most of these and other problems were corrected by BYU (not WES), and we believe our interaction with BYU has the potential to greatly improve the GMS (if the fixes to the bugs we found are in fact carried into new versions of GMS).

Appendix 2: Sources for hydrologic data used in this research

Type of Data	Site name	Responsible Agency
canal stage and discharge	S-174	SFWMD
canal stage and discharge	S-175	SFWMD
canal stage and discharge	S-176	SFWMD (gated weir)
canal stage and discharge	S-176	ENP (AVM)
canal stage and discharge	S-177	SFWMD
canal stage and discharge	S-332	SFWMD
stage and discharge ¹	TSB	ENP
rainfall	S-174	SFWMD
rainfall	S-177	SFWMD
rainfall	S-332	SFWMD
rainfall	ROBL	ENP
rainfall	RPL	ENP
evaporation	TAMITR40	NOAA
groundwater head ²	G789	USGS
groundwater head ²	G613	USGS
groundwater head ²	R158	ENP
groundwater head ²	R3110	ENP
groundwater head ²	CR2	
groundwater head	E112	
groundwater head	NTS1	
groundwater head	NTS10	• .
groundwater head	FRGPD1	
groundwater head	FRGPD2	
groundwater head	FROGP	
groundwater head	ROBL	

Notes

SFWMD = South Florida Water Management District

ENP = Everglades National Park

NOAA = National Oceanic and Atmospheric Administration

USGS = Unites States Geological Survey

- 1. Could be considered surface water or groundwater head, depending on whether water level at the gauge is above or below ground surface (usually it was above); water levels above ground surface were used with a rating curve for Taylor Slough to calculate discharge in the slough.
- 2. Well was on the boundary of the model domain, and head data were used as boundary condition; data from other wells in the interior of the model domain was used in comparison of observed and modeled head.

Appendix 3: Water quality data used in this research Chloride concentrations in mM

	Chloride co	ncentration	s in mM		t _a			
	C113	S174H	S174T	S175H	S175T	S176H	S176T	S176avm
09/07/1996	0.971		1.141	0.918				0.929
11/06/1996	0.809	1.034	1.039	0.9	0.879	1.049	0.892	
12/04/1996	1.058	1.078	0.881	0.706	0.839	1.099	1.104	
01/09/1997	1.437		1.5	0.868			1.491	
01/21/1997	1.082		0.932	0.897			1.139	
02/12/1997	1.762		0.949	0.912			1.946	
02/26/1997	1.716		1.743				1.752	
03/12/1997	2.213		2.225				2.226	
03/25/1997	1.627		1.637	1.039			1.652	
04/08/1997	2.219		2.266	2.193			2.25	
04/25/1997	2.293		2.217	2.097			2.339	
05/08/1997	1.508	2.021	1.081	1.573		1.987	1.703	
05/21/1997	1.457	2.059	1	1.232		2.057	1.474	
06/11/1997	1.205	2.000	1.257	0.645		2.007	1.261	
06/24/1997	1.098		1.218	0.99		1.227	1.136	
07/08/1997	1.094		1.157	1.052		1.158	1.087	1.082
07/24/1997	1.106		1.198	1.003	0.977	1.208	1.14	1.096
08/07/1997	1.047		1.164	0.947	0.947	1.169	1.05	1.047
08/20/1997	1.066		1.161	1.034	0.995	1.183	1.062	1.056
09/03/1997	1.026		1.213	0.987	0.995	1.100	1.19	1.096
09/17/1997	1.052		1.206	0.95			1.198	1.090
09/30/1997	1.112		1.189	1.044			1.155	1.119
10/15/1997	1.028		1.253	1.066		1.26	1.124	1.119
10/13/1997	1.216		1.299	1.182		1.20	1.124	1.203
11/12/1997	1.210	1.126	1.059	0.925		1.136	1.081	0.972
11/26/1997	1.329	1.120	1.342	1.439		1.130		
12/10/1997	1.087		1.342	1.459	1 020	1 207	1.343	1.34
12/10/1997	0.949				1.038	1.207	1.088	1.091
01/07/1998	0.896		1.123 1.202	0.974	0.954	1.139	0.945	0.951
01/07/1998	0.696	1.183	0.928	0.982 0.953	0.969	1.178	0.92	0.886
02/04/1998	0.955	1.103			0.954	1.17	0.958	0.954
02/04/1998	1.023		1.008	0.874			1.021	0.97
03/05/1998	1.292		1.129 1.35	1.003	4 240		1.129	1.136
03/19/1998	1.108		1.304	1.082 1.174	1.318 1.17		1 201	0.988
04/01/1998	1.061		1.304	1.174		1 21	1.291 1.162	1.248
04/01/1998	1.199				1.183	1.31		1.257
04/10/1998			1.751	1.474	1.39		1.749	1.633
05/12/1998	0.861		1.217	1.298	1.293	1 211	1.214	1.19
05/12/1998	1.296		1.305	1.354	1.311	1.311	1.265	1.297
	1.215	4 504	1.709	1.555	1.471	1.712	1.554	1.38
06/10/1998	1.526	1.561	1.563	1.4	1.374		1.508	1.548
06/24/1998	1.488	1.471	1.445	1.464	1.45		1.47	1.465
07/08/1998	1.611	1.633	1.387	1.383	1.369		1.64	1.594
07/22/1998	1.271	1.267	1.014	1.208	1.208		1.265	1.268
08/07/1998	1.099		1.293	1.071	1.076	4.400	1.283	1.175
08/22/1998	1.135	4.450	1.145	1.128	1.123	1.136	1.144	1.155
09/03/1998	1.04	1.156	1.142	1.063	1.111	1.163	1.066	1.039
09/17/1998	0.98		1.079	0.826		4 404	1.1	1.076
10/01/1998	1.031		1.1	0.947		1.104	1.052	1.038
10/15/1998	0.95		1.09	0.981	0.947	1.112	1.033	0.962

10/29/1998	0.94		1.109	1.025	0.988	1.1	1.054	0.95
11/12/1998	0.923		1.086	1.004	0.979	1.072	1.024	0.94
11/24/1998	1.161		0.973	1.101	1.15	1.01	0.989	0.889
12/10/1998	0.968		1.067	0.995	1.015		1.016	0.975
12/23/1998			1.065	0.988		1.048	0.948	0.912
01/06/1999	0.943		1.074	1.081		1.08	0.967	0.933
01/21/1999	0.956		1.214	1.151	1.142	1.19	0.989	0.923
02/04/1999	1.008	1.227	1.21	1.195	1.111	1.214	1.005	0.992
02/18/1999	1.013	1.266	0.992	1.105	1.086	1.266	1.035	1.014
03/04/1999	1.326	1.003	1.364	0.888	1.048		1.338	1.355
03/18/1999	1.617		1.649	1.212	1.102		1.615	1.601
04/01/1999	1.429		1.455	1.52	1.488		1.437	
04/15/1999	1.358		1.373	1.519	1.488		1.346	1.367
04/29/1999	1.53	1.549	1.526	1.43	1.343		1.535	1.524
05/13/1999	1.684	1.741	1.484	1.489	1.378	1.651	1.703	1.657
05/27/1999	1.451		1.631	1.136	1.158	1.619	1.463	1.457
06/10/1963	1.201		1.322	1.283	1.229	1.328	1.209	1.197
06/24/1999	1.231		1.279	1.2			1.297	1.255
07/09/1999	1.249		1.222	1.186		1.26	1.253	1.259
07/22/1999	1.052		1.222	1.085	1.107	1.225	1.054	1.038
08/19/1999	0.987		1.16	1.108	1.081	1.158	0.998	0.988
09/23/1999	0.989		1.076	0.933		1.072	1.019	1.006
10/26/1999	0.948	0.968	0.965	0.732			0.975	0.959
12/01/1999	0.912		0.99	0.945			0.989	0.957
01/12/2000	1.001		0.991	1.199			1.285	1.09

	S177H	S177T	S178H	S178T	S332	P3surf	P3S	P3D
09/07/1996	01//11	0.922	1.179	1.147	0002		0.547	0.612
11/06/1996	0.785			1.177			0.648	0.654
12/04/1996		0.023		1.026			0.6	0.00.
01/09/1997		1.257	1.573	1.020			0.619	0.62
					0.874		0.581	0.594
01/21/1997		1.145			1.005		0.631	0.629
02/12/1997		1.573	1.461		0.858		0.653	0.626
02/26/1997		1.703					0.658	0.676
03/12/1997		2.162	1.615		1.62			0.685
03/25/1997		1.485			0.95	•	0.716	
04/08/1997		2.28			2.457		0.822	0.744
04/25/1997		2.042	2.015		2.056		1.408	0.904
05/08/1997	1.768		1.986		1.396		1.423	1.255
05/21/1997	1.354		1.56		0.943		1.348	1.289
06/11/1997		1.158	0.961		0.631		0.985	1.074
06/24/1997		0.963	1.033		0.961		0.873	0.96
07/08/1997		0.949	1.129		1.049		0.693	0.658
07/24/1997		0.966	1.043	1.076			0.719	0.685
08/07/1997		0.878	0.951	1.053	0.947		0.652	0.647
08/20/1997		0.862	1.062	1.021	1.099		0.666	0.572
09/03/1997		1.024	0.866		0.955		0.625	0.642
09/17/1997		1.008	0.986		1.039		0.621	0.627
09/30/1997		1.036	1.061		1.073		0.659	0.688
10/15/1997	0.956	1.033	1.186		1.141		0.608	0.617
10/29/1997	0.889	1.007	1.191		1.15		0.591	0.647
11/12/1997	0.744	0.83	1		0.857		0.53	0.534
11/26/1997		1.199	1.102		1.219		0.672	0.738
12/10/1997		0.984	1.098		1.007	0.568	0.689	0.74
12/20/1997		0.903	0.982		0.972	0.477	0.629	0.644
01/07/1998	1.005	0.922	0.96	0.954	1.035		0.586	0.611
01/22/1998	0.876		0.961		0.756		0.594	0.614
02/04/1998		0.911	0.668		0.834		0.607	0.614
02/18/1998	0.805		0.813	0.913	1.088		0.522	0.544
03/05/1998		0.95	0.785	0.912	1.234		0.567	0.626
03/19/1998		1.132	0.767	0.908	1.251		0.606	0.667
04/01/1998		0.961	0.898	0.908	1.274		0.645	0.663
04/16/1998		0.93	0.929	0.872	1.78		0.853	0.877
04/30/1998		1.165	1.17	1.253	1.253		1.152	1.13
05/12/1998		1.265	1.134	1.267	1.264		1.193	1.159
05/27/1998		1.197	1.268	1.073	1.712		1.272	1.224
06/10/1998	0.969	0.977	1.178	0.97	1.385		1.46	1.267
06/24/1998	0.000	1.457	1.778	1.022	1.496		1.433	1.278
07/08/1998	1.563	1.504	1.133	1.104	1.231		1.39	1.218
07/22/1998	7.000	1.211	0.977	1.066	1.015		1.167	1.142
08/07/1998		1.134	0.732	0.912	0.991		1.066	0.912
08/22/1998		1.073	0.971	0.991	1.058		0.988	0.796
09/03/1998	0.949	1.062	1.036	1.01	1.001		0.965	0.779
09/03/1998	0.543	0.919	0.638	1.01	0.82		0.823	0.656
10/01/1998		0.963	0.030		0.933		0.874	0.788
10/01/1998		0.869	0.923	0.879	0.937		0.8	0.695
10/10/1990		0.009	0.340	0.073	0.001		0.0	0.500

10/29/1998		0.93	0.992	0.895	1.033	0.779	0.689
11/12/1998		0.941	0.916	0.884	0.918	0.741	0.653
11/24/1998	0.879	0.902	0.98	1.002		0.741	0.669
12/10/1998	0.894	0.917	0.986	0.881	1.019	0.725	0.653
12/23/1998	0.927	0.893	0.904		0.995	0.182	0.656
01/06/1999		0.913	1.019	0.911		0.702	0.711
01/21/1999		0.943	1.006	0.966	1.159	0.756	0.765
02/04/1999	0.974	0.978	1.073	0.948	1.15	0.766	0.778
02/18/1999	1.137	0.98	1.085	0.953	1.095	0.804	0.807
03/04/1999	1.09	1.024	1.211	0.966	0.811	0.735	0.75
03/18/1999		1.368	1.267	1.03	1.251	0.721	0.742
04/01/1999		1.535	1.343	1.54		0.788	0.889
04/15/1999		1.39	1.684	1.657	1.442	0.862	1.131
04/29/1999		1.47	1.894	1.385	1.407	1.018	1.004
05/13/1999	1.637	1.666	1.035	1.436	1.499	1.136	1.059
05/27/1999	1.427	1.502	0.968	1.093	1.141	1.104	1.061
06/10/1963	1.131	1.182	0.969	1.002	1.266	1.099	1.148
06/24/1999		1.072	0.937	0.957	1.202	1.14	1.107
07/09/1999		1.047	1.023	0.997	1.146	1.041	1.063
07/22/1999	1.056	1.037	0.913	1.054	1.105	0.919	0.849
08/19/1999	0.937	0.99	1.002	0.94	1.037	0.933	0.794
09/23/1999		0.914	0.873	0.849	0.894	0.795	0.887
10/26/1999		0.91	0.709	0.842	0.715	0.604	0.691
12/01/1999		0.923	0.896		0.963	0.747	0.766
01/12/2000		1.19	0.974	0.925	1.21	0.802	0.863

	P9S	P9D	P10S	P10D	P20S	P20D	P21S	P21D
00/07/1006					F203	1200	1210	1210
09/07/1996				0.525				
11/06/1996								
12/04/1996			0.527					
01/09/1997								
01/21/1997				0.52				
02/12/1997								
02/26/1997				0.526				
03/12/1997								
03/25/1997				0.524				
04/08/1997								
04/25/1997				0.537				
05/08/1997				0.526				
05/21/1997				0.52				
06/11/1997				0.512				
06/24/1997	0.302	0.414		0.423				
07/08/1997	0.407	0.427	0.333	0.452				
07/24/1997	0.402	0.431	0.414	0.438				
08/07/1997	•							
08/20/1997	0.385	0.394	0.284	0.405				
09/03/1997	0.524	0.421	0.648	0.415				
09/17/1997	0.746	0.538	0.857	0.462				
09/30/1997	•		0.972	0.581				
10/15/1997	0.799	0.628	0.889	0.479				
10/29/1997	0.775	0.561	0.83	0.464				
11/12/1997	•		0.699	0.379			0.506	6
11/26/1997	•		0.756	0.448	0.84	2	0.593	3
12/10/1997	•		0.715	0.481	0.77	4 0.86	0.595	0.661
12/20/1997			0.693	0.475	0.76	5 0.837	0.534	0.615
01/07/1998	ı		. 0.6	0.489	0.78	8 0.843	0.54	0.613
01/22/1998			0.584	0.517	0.73	2 0.841	0.553	0.626
02/04/1998			0.584	0.499	0.75	9 0.823	0.545	0.616
02/18/1998			0.538	0.469	0.79	6 0.828	0.532	0.609
03/05/1998			0.525	0.466	0.8	1 0.832	0.593	0.603
03/19/1998			0.515	0.468	0.81	5 0.844	0.567	0.599
04/01/1998			0.518	0.475	0.81	5 0.826	0.559	0.591
04/16/1998			0.5	0.477	0.838	8 0.86	0.552	0.593
04/30/1998			0.495	0.488	0.84		0.567	0.607
05/12/1998			0.495	0.483	0.84			0.638
05/27/1998			0.496	0.477	0.848			
06/10/1998			0.515	0.485	0.85			
06/24/1998			0.509	0.51	0.848			
07/08/1998			0.516	0.497	0.866			
07/22/1998			0.525	0.485	0.85		0.635	
08/07/1998		•	0.552	0.479	0.88			
08/22/1998			0.529	0.481	0.854			
09/03/1998			0.537	0.498	0.859			
09/03/1998			0.545	0.450		? ?	0.488	
10/01/1998			0.251	0.504	0.843			
10/01/1998			0.712	0.499	0.743			
10/13/1990			0.7 12	U. 4 33	0.74	0.000	0.004	0.000

10/29/1998	0.72	0.546	0.819	0.862	0.638	0.852
11/12/1998	0.785	0.621	0.799	0.849	0.667	0.809
11/24/1998	0.721	0.621	0.812	0.892	0.709	0.806
12/10/1998	0.718	0.623	0.838	0.887	0.782	0.744
12/23/1998	0.687	0.622	0.852	0.883	0.73	0.757
01/06/1999	0.686	0.641	0.829	0.887	0.735	
01/21/1999	0.746	0.69	0.934	0.973	0.773	0.819
02/04/1999	0.745	0.684	0.959	1.01	0.785	0.798
02/18/1999	0.719	0.674	0.908	1.006	0.704	0.781
03/04/1999	0.723	0.639	0.921	1.006	0.814	0.802
03/18/1999	0.715	0.639	0.925	1.006	0.813	0.823
04/01/1999	0.698	0.667	0.91	0.989	0.803	0.792
04/15/1999	0.679	0.876	0.942	0.999	0.797	0.792
04/29/1999	0.408	1.063	0.956	0.998	0.787	0.793
05/13/1999	0.698	1.092	1.009	1.019	0.785	0.758
05/27/1999	0.702	0.885	0.983	1.051	0.806	0.789
06/10/1963	0.767	0.734			0.782	1.05
06/24/1999	0.783	0.679	1.059	1.022	0.795	0.794
07/09/1999	0.797	0.612	1.024	1.052	0.755	0.788
07/22/1999	0.765	0.79	0.574	0.738	0.685	0.717
08/19/1999	0.698	0.609	1.056	1.087	0.759	0.84
09/23/1999	0.939	0.563			0.742	0.799
10/26/1999	0.738	0.591				0.826
12/01/1999	0.833	0.731			0.775	0.82
01/12/2000	0.925	0.922			0.812	0.863

	P22S	P22D	P23S	P23D	USGS-S	USGS-I
09/07/1996			. 200			0.585
11/06/1996						0.758
12/04/1996						0.719
01/09/1997						0.748
01/03/1997						0.712
01/21/1997						0.724
02/12/1997						0.712
02/20/1997						0.712
03/12/1997						0.718
03/25/1997						0.720
04/06/1997	*					0.733
05/08/1997						0.722
05/06/1997						0.722
05/21/1997		•				0.734
06/11/1997						0.705
07/08/1997						0.703
						0.681
07/24/1997 08/07/1997					-	0.647
						0.636
08/20/1997						0.635
09/03/1997						0.612
09/17/1997						0.653
09/30/1997						0.647
10/15/1997						0.639
10/29/1997					0.424	0.055
11/12/1997	0.000	0.00			0.424	0.632
11/26/1997	0.809		4.042	0.000	0.474	0.607
12/10/1997	0.789		1.013	0.998 0.857	0.474	0.553
12/20/1997	0.698		0.847	0.805	0.425	0.555
01/07/1998	0.679		0.766 0.801	0.803	0.423	0.53
01/22/1998 02/04/1998	0.78 0.665		0.801	0.801	0.427	0.531
02/04/1998	0.626		0.773	0.703	0.399	0.508
03/05/1998	0.020		0.818	0.705	0.415	0.509
03/03/1998	0.569		1.019	1.006	0.415	0.507
04/01/1998	0.566		1.009	1.016	0.426	0.503
04/01/1998	0.574		1.196	1.183	0.453	0.487
04/30/1998	0.577		1.130	1.258	0.498	0.466
05/12/1998	0.577		1.236	1.237	0.468	0.479
05/12/1998	0.573	0.544	1.288	1.271	0.48	0.49
06/10/1998	0.575		1.526	1.465	0.479	0.494
06/24/1998	0.57		1.475	1.447	0.47	0.493
07/08/1998	0.569		1.46	1.425	0.473	0.49
07/22/1998	0.009		1.439	1.418	0.475	0.49
08/07/1998	0.601	0.608	1.391	1.395	0.475	0.51
08/22/1998	0.605		1.283	1.308	0.481	0.513
09/03/1998	0.603		1.167	1.187	0.498	0.476
09/03/1998	0.587		1.118	1.138	0.430	0.325
10/01/1998	0.587		1.073	1.148	0.435	0.498
10/01/1998	0.573		0.957	1.028	0.422	0.497
10/10/1990	0.010	0.020	0.001	1.020	J. :44	357

10/29/1998	0.582	0.661	0.893	0.979	0.43	0.496
11/12/1998	0.59	0.669	0.902	0.991	0.427	0.479
11/24/1998	0.604	0.697	0.938	0.992	0.44	0.491
12/10/1998	0.613	0.728	0.912		0.455	0.494
12/23/1998	0.609	0.699	0.919	0.971	0.443	0.475
01/06/1999	0.604	0.709	0.924	0.973	0.443	0.485
01/21/1999	0.654	0.756	1.067	1.023	0.478	0.505
02/04/1999	0.658	0.775	1.116	1.146	0.493	0.519
02/18/1999	0.788	0.704	0.743	1.141	0.481 ?	
03/04/1999	0.657	0.79	0.912	1.043	0.5	0.519
03/18/1999	0.66	0.783	0.823	0.996	0.5	0.518
04/01/1999	0.653	0.744	0.8	0.903	0.486	0.52
04/15/1999	0.661	0.755	0.808	0.887	0.48	0.507
04/29/1999	0.682	0.73	0.803	0.874	0.491	0.508
05/13/1999	0.684	0.724	0.831	0.882	0.501	0.518
05/27/1999	0.679	0.699	0.857	0.933	0.507	
06/10/1963	0.662	0.701	0.854		0.493	0.523
06/24/1999	0.657	0.718	0.84	0.946	0.487	0.523
07/09/1999	0.667	0.728	0.778	0.866	0.501	0.522
07/22/1999	0.792	0.858	0.494	0.505		
08/19/1999	0.689	0.729	0.87	0.878	0.53	0.524
09/23/1999	0.612	0.662	0.915	0.912	0.496	0.542
10/26/1999	0.639	0.68	0.69	0.738	0.374	0.568
12/01/1999	0.677	0.71	0.642	0.675	0.483	0.556
01/12/2000	0.669	0.714	0.639	0.684	0.483	0.56